Kinetics of fluid demixing in complex plasmas

Morphological Data Analysis using Minkowski Tensors

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Outline

1. Minkowski Valuations

2. Elementary Applications

3. Simulated demixing of a binary complex plasma

4. Outlook

Brezen!

Fig. 1 : Above: a Bavarian brezen ("pretzel")

$$W_2(K) = \#(\mathit{connected\ regions}) - \#(\mathit{holes}) \tag{1}$$

Minkowski Functionals

For a body K with a smooth boundary contour ∂K embedded in D -dim euclidean space the $D+1$ Minkowski functionals are defined as:

- $W_0(K) \;=\; \int_K \mathrm{d}^D r$
- $W_\nu(K) \;=\; \int_{\partial K} G_\nu(r)\,\mathrm{d}^{D-1} r \qquad , \qquad 1 \leq \nu \leq D$

$G_\nu(r)$ are the elementary symmetric polynomials of the local principal curvatures.

in 2d:

- $W_0(K) \;=\; \int_K \mathrm{d}^2 r \qquad \propto \#(\mathit{pixels})$ (area)
- $W_1(K) \;=\; \int_{\partial K} \mathrm{d}r \qquad \propto 2\#(\mathit{edges}) - 4\#(\mathit{squares})$ (circumference)
- $W_2(K) \;=\; \int_{\partial K} \kappa(r)\,\mathrm{d}r \qquad \propto 2\#(\mathit{edges}) - 4\#(\mathit{squares})$ (euler characteristic)

similar in 3d:

- $W_0(K) = \int_K \mathrm{d}^3 r$ (volume)
- $W_1(K) = \int_{\partial K} \mathrm{d}^2 r$ (area)
- $W_2(K) = \int_{\partial K} \kappa_1 + \kappa_2\, \mathrm{d}^2 r$ (integrated mean curvature)
- $W_3(K) = \int_{\partial K} \kappa_1 \kappa_2\, \mathrm{d}^2 r$ (euler characteristic)

Poperties and applications

MFs are motion invariant, additive, continuous. They form a complete family of morphological measures. They are sensitive to higher order correlations.

Applications:

- curvature energy of membranes
- order parameter in Turing patterns
- density functional theory for fluids (as hard balls or ellipsoids)
- test point distributions (find clusters, filaments, underlying pointprocess)
- non-gaussianity of CMB

Abstraction to tensor valued valuations

In order to account also for directional properties it is natural to abstract the scalar valued MF to tensor valued quantities called MT:

Definition

- $W_0^{a,0}(K) \;:=\; \int_K \mathrm{d}^D r \;\; \mathbf{r}^{\odot a} \qquad , \qquad (\nu = b = 0)$
- $W_\nu^{a,b}(K) \;:=\; 1/D \int_{\partial K} \mathrm{d}^{D-1} r \;\; G_\nu(r) \;\; \mathbf{r}^{\odot a} \odot \mathbf{n}^{\odot b} \qquad , \qquad (\nu, b \neq 0)$

Properties:

- They are isometry covariant, i.e their behaviour under translation and rotation is given by:

$$W_\nu^{a,b}(K + \mathbf{t}) \;=\; \sum_{i=0}^{a} \binom{a}{i} \mathbf{t}^i \, W_\nu^{a-i,b}(K) \tag{2a}$$

$$W_\nu^{a,b}(\hat{O}\, K) \;=\; \hat{O}_{a+b}\, W_\nu^{a,b}(K) \tag{2b}$$

- They are additive: $W_\nu^{a,b}(K_1 \cup K_2) = W_\nu^{a,b}(K_1) + W_\nu^{a,b}(K_2) - W_\nu^{a,b}(K_1 \cap K_2)$

- They are homogeneous: $W_\nu^{a,b}(\lambda K) \;=\; \lambda^{3+a-\nu}\; W_\nu^{a,b}(K)$

Completeness

Let K^d denote the family of all compact convex subsets of the Euclidean space R^d . Let L be a linear space.

Definition

A function $\phi : K^d \to L$ is called a valuation if

$$\phi(K_1 \cup K_2) + \phi(K_1 \cap K_2) = \phi(K_1) + \phi(K_2) \tag{3}$$

for any $K_1, K_2 \in K^d$ such that $K_1 \cup K_2 \in K^d$

Theorem (Alesker 1999)

Let $\phi : K^d \to L$ be a continuous translation- and $SO(d)$-covariant valuation. Then ϕ has the form

$$\phi(K) = \sum_j c_j W_j(K) \tag{4}$$

where $W_j(K)$ is the j^{th} Minkowski valuation, and $c_j \in L$ are fixed uniquely defined vectors.

- every morphological measure is a linear combination of Minkowski valuations

Isotropy measure β

For a body K and each Minkowski tensor $W_\nu^{a,b}(K)$ an isotropy index can be defined as the ratio between smallest and largest eigenvalue of the *DxD*-Matrix representing each Minkwoski tensor.

Definition

$$\beta_\nu^{a,b}(K) := \frac{\lambda_{min}\left(W_\nu^{a,b}(K)\right)}{\lambda_{max}\left(W_\nu^{a,b}(K)\right)} \tag{5}$$

The dimensionless isotropy index is a pure shape measure. It is invariant under isotropic scaling of K.

examples:

- sphere, circle $\beta = 1$
- cube, square $beta = 1$
- box $\beta = shorter/longer\ edge$

$\Rightarrow$ isotropy measure in the sense of elongation

Consider the simplest rank 4 MT: $W_1^{04}(K) \;=\; 1/3 \cdot \int_{\partial K} \mathrm{d}^2 r \;\; \mathbf{n}(\mathbf{r}) \otimes \mathbf{n}(\mathbf{r}) \otimes \mathbf{n}(\mathbf{r}) \otimes \mathbf{n}(\mathbf{r})$

- translation invariant
- symmetric $\left(W_1^{04}\right)_{ijkl} \;=\; \left(W_1^{04}\right)_{(ijkl)} \;\Rightarrow\;$ 15 independent elements in 3d

Rewrite W_1^{04} in the Mehrabadi supermatrix notation as a 6×6 matrix:

$$M = \begin{pmatrix} S_{xxxx} & S_{xxyy} & S_{xxzz} & \sqrt{2}\,S_{xxyz} & \sqrt{2}\,S_{xxxz} & \sqrt{2}\,S_{xxxy} \\ S_{xxyy} & S_{yyyy} & S_{yyzz} & \sqrt{2}\,S_{yyyz} & \sqrt{2}\,S_{yyxz} & \sqrt{2}\,S_{yyxy} \\ S_{xxzz} & S_{yyzz} & S_{zzzz} & \sqrt{2}\,S_{zzyz} & \sqrt{2}\,S_{zzxz} & \sqrt{2}\,S_{zzxy} \\ \sqrt{2}\,S_{xxyz} & \sqrt{2}\,S_{yyyz} & \sqrt{2}\,S_{zzyz} & 2\,S_{yzyz} & 2\,S_{yzxz} & 2\,S_{yzxy} \\ \sqrt{2}\,S_{xxxz} & \sqrt{2}\,S_{yyxz} & \sqrt{2}\,S_{zzxz} & 2\,S_{yzxz} & 2\,S_{xzxz} & 2\,S_{xzxy} \\ \sqrt{2}\,S_{xxxy} & \sqrt{2}\,S_{yyxy} & \sqrt{2}\,S_{zzxy} & 2\,S_{yzxy} & 2\,S_{xyxz} & 2\,S_{xyxy} \end{pmatrix}$$

with $S = W_1^{04}(K)/W_1(K)$

It is possible to define a distance measure on the space of bodies:

Definition

$$\Delta(K_1, K_2) := \left(\sum_{i=1}^{6} \left(\zeta_i(K_1) - \zeta_i(K_2)\right)^2 \right)^{1/2} \tag{7}$$

It is a pseudometric. It is symmetric, the triangle inequality holds, but:

$\Delta(K_1, K_2) = 0 \Leftarrow K_1 = K_2$

Symmetry pseudometric Δ

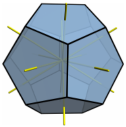
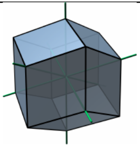
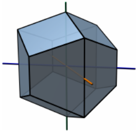
structure	ico	fcc	hcp	bcc	sc
type	(5,1)	(3,2,1)	(2,2,1,1)	(3,2,1)	(3,2,1)
ς_1	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$
ς_2	$\frac{2}{15}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{8-4/\sqrt{3}}{33}$	$\frac{1}{3}$
ς_3	$\frac{2}{15}$	$\frac{1}{6}$	$\frac{5}{36}$	$\frac{8-4/\sqrt{3}}{33}$	$\frac{1}{3}$
ς_4	$\frac{2}{15}$	$\frac{1}{6}$	$\frac{5}{36}$	$\frac{8-4/\sqrt{3}}{33}$	0
ς_5	$\frac{2}{15}$	$\frac{1}{12}$	$\frac{1}{9}$	$\frac{-1+2\sqrt{3}}{33}$	0
ς_6	$\frac{2}{15}$	$\frac{1}{12}$	$\frac{1}{9}$	$\frac{-1+2\sqrt{3}}{33}$	0
					

Fig. 2 : Above: eigenvalue tuple for ideal polyhedra, Kapfer 2011

Ideal crystal with noise

Rank 2 β MT analysis for ideal hcp, fcc, bcc data with gaussian noise. → **Isotropy inedx drops exponentially with increasing noise, independent of crystal type.**

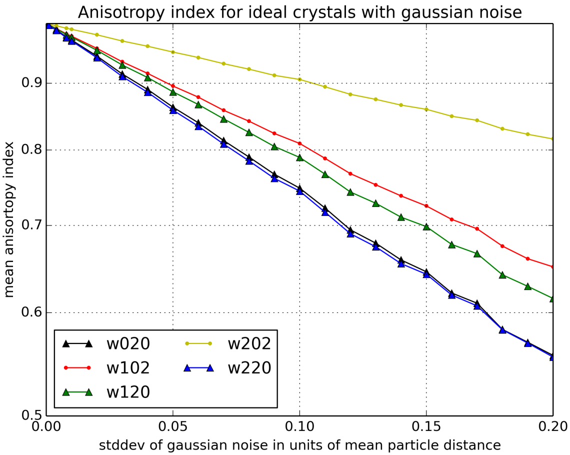
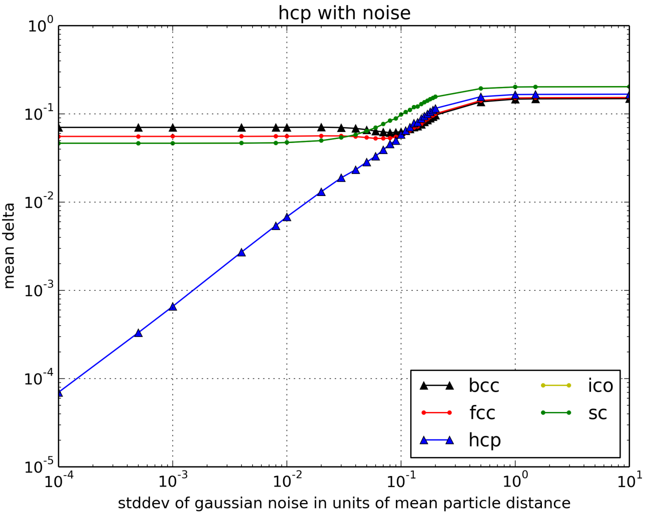


Fig. 3 : Above: Isotropy index drops exponentially with increasing noise.

Ideal crystal with noise

Rank 4 Δ MT analysis for ideal hcp data with gaussian noise.



Simulated demixing of a binary complex plasma

Plasma conditions:

- stationary isotropic highly collisional plasma
- Plasma production due to electron impact ionization
- Plasma losses due to three-body bulk recombination and ambipolar diffusion to the plasma boundaries.

The continuity and momentum equations for e.g. ions are:

$$\begin{aligned} \nabla(n_i v_i) &= \nu_I n_e - \nu_L n_i - \beta n_e n_i \\ (v_i \nabla) v_i &= -(e/m_i)\nabla\Phi - (u_{T_i}^2/n_i)\nabla n_i - \nu_i v_i \end{aligned} \qquad (8)$$

(here v_i and m_i are the velocity and mass of the ions, ν_I the ionization frequency, ν_L the characteristic frequency of ambipolar losses,β the recombination coefficient, ν_i the characteristic frequency of ion-neutral collisions, Φ the electrical potential, and u_{T_i} is the ion thermal velocity.)

Solving the Poisson equation leads to a double Yukawa repulsive potential:

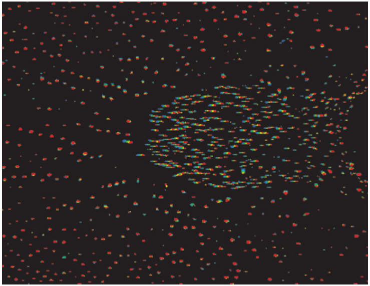
$$\Phi(r) \;=\; 1/r \cdot \left(Z_{SR}^* \exp(-r/\lambda_{SR}) + Z_{LR}^* \exp(-r/\lambda_{LR})\right) \qquad (9)$$

Simulation:

- $\Lambda \;=\; \lambda_{LR}/\lambda_{SR}$ as measure for dominance of LR over SR interaction
- demixing is accompanied by domain growth $L(t) \propto t^{\alpha}$

Simulated demixing of a binary complex plasma

[pk3-plus]



[simulation]

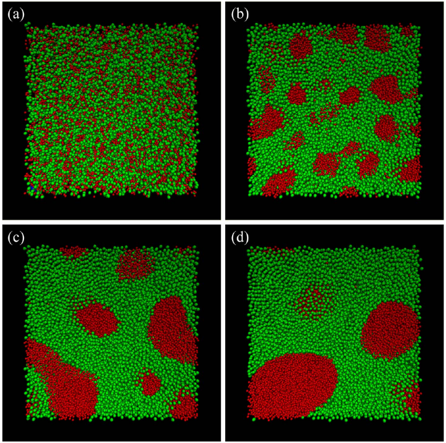


Fig. 5 : Above: Demixing of a binary complex plasma. Ivlev,2009 and Jiang,2011.

Simulated demixing of a binary complex plasma

Histogram method to get the number of particles in a demixed domain:

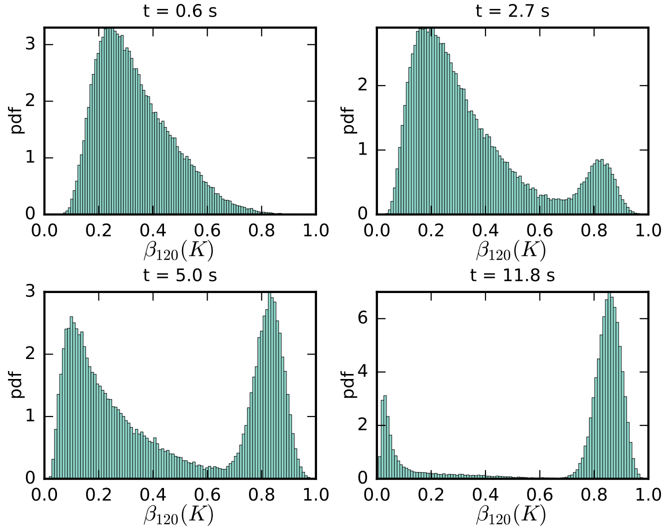


Fig. 6 : Above: Growth of minority phase domains for simulated demixing of a complex plasma.

Simulated demixing of a binary complex plasma

Domain growth for measures $m \in \{MT0, MT2, power\ spectum\ method\}$.

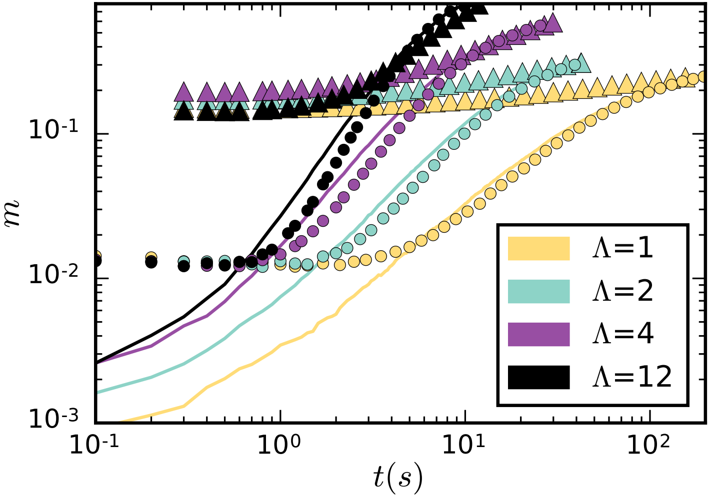


Fig. 7 : Above: Growth of minority phase domains for simulated demixing of a complex plasma. Lines show MT0 analysis, circles MT2 analysis and triangles a power spectrum method.

Simulated demixing of a binary complex plasma

Slopes of MT measures hints towards universal behavior:

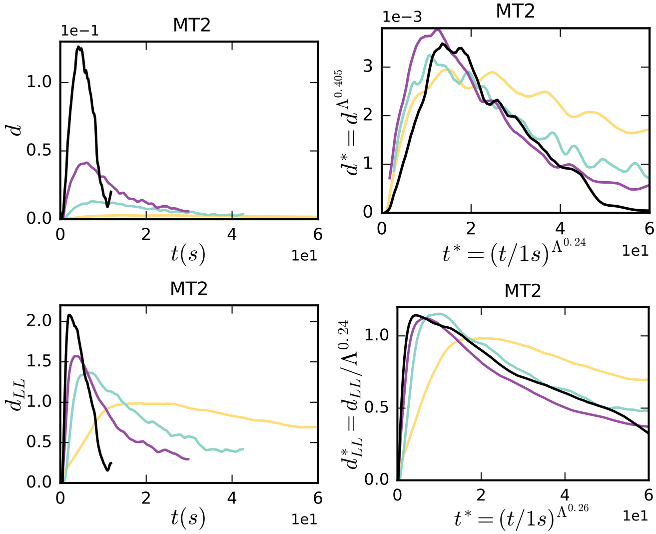


Fig. 8 : Above: Universal behaviour of gradients of MT measures for $\Lambda \neq 1$.

Simulated demixing of a binary complex plasma

Demixing occurs in two stages:

- agglomeration of neighbouring particles
- cascades of merging domains (only for $\Lambda > 1$)

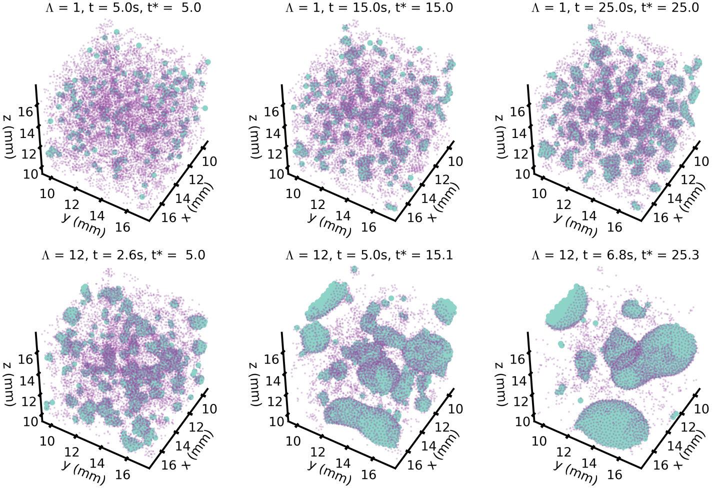


Fig. 9 : Above: Qualitative differences in demixing behavior for $\Lambda > 1$.

Outlook

- investigate transition close to $\Lambda = 1$
- MT demixing analysis of well know Lennard Jones system
- demixing for general interaction potentials, universality?

Thank you for your attention!